

## Supplementary Materials

These supplementary materials present proofs of Theorems 2, 3, 4, and 5. First, we derive Theorem 2 as explained hereinafter.

**Theorem 2** Under Assumption 1, let  $G^*(\mathbf{V})$  be the true structure. I-maps NPCDAG with the fewest NCP are classification equivalent to  $G^*(\mathbf{V})$ .

**Proof** Let  $G_{NPC}^*(\mathbf{V})$  be an NPCDAG that is classification equivalent to  $G^*(\mathbf{V})$ . This theorem can be proven by contradiction. Assuming that there exists an I-map NPCDAG  $G'$  with the fewest NCP which is not classification equivalent to  $G_{NPC}^*(\mathbf{V})$ , then because  $G'$  has the fewest NCP in I-maps NPCDAG,  $G'$  represents some d-separations related with the class variable which  $G_{NPC}^*(\mathbf{V})$  does not represent. Such d-separations are also not represented by  $G^*(\mathbf{V})$  because  $G^*(\mathbf{V})$  is classification equivalent to  $G_{NPC}^*(\mathbf{V})$ . This lack of representation contradicts that  $G'$  is an I-map, which completes the proof.  $\square$

Next, we introduce the following theorem and definitions.

**theorem** (Local independences in Bayesian networks) (Pearl 2000)

Letting  $G = (\mathbf{V}, \mathbf{E})$  be a Bayesian network structure, and letting  $\mathbf{ND}_G(X)$  be a set of non-descendants of  $X$ , then the following holds:

$$\forall X \in \mathbf{V}, D_{sep}_G(X, (\mathbf{ND}_G(X) \setminus \mathbf{Pa}_X^G) \mid \mathbf{Pa}_X^G).$$

**Definition** (Asymptotic consistency of scoring criterion) (Chickering 2002)

Let  $G_1 = (\mathbf{V}, \mathbf{E}_1)$ , and  $G_2 = (\mathbf{V}, \mathbf{E}_2)$  be the structures. A scoring criterion  $Score$  has asymptotic consistency if the following two properties hold when the sample size is sufficiently large.

- If  $G_1$  is an I-map and  $G_2$  is not an I-map, then  $Score(G_1) > Score(G_2)$ .
- If  $G_1$  and  $G_2$  both are I-maps and if  $G_1$  has fewer parameters than  $G_2$ , then  $Score(G_1) > Score(G_2)$ .

**Definition** (Asymptotic local consistency of scoring criterion) (Chickering 2002)

Let  $G_1 = (\mathbf{V}, \mathbf{E}_1)$  be any structure. Also, let  $G_2$  be the structure which results from adding edge  $Y \rightarrow X$ . A scoring criterion  $Score$  has an asymptotic local consistency if

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the following two properties hold when the sample size is sufficiently large.

- $I(X, Y \mid \mathbf{Pa}_X^{G_1}) \Rightarrow Score(G_1) > Score(G_2)$ .
- $\neg I(X, Y \mid \mathbf{Pa}_X^{G_1}) \Rightarrow Score(G_1) < Score(G_2)$ .

To derive Theorem 3, we introduce the following lemma.

**Lemma 1** Assuming disjoint variable sets  $\mathbf{X}, \mathbf{Y}, \mathbf{A}, \mathbf{B}$ , then the following holds.

$$\neg I(\mathbf{X}, \mathbf{Y} \mid \mathbf{A}) \Rightarrow \neg I(\mathbf{X}, \mathbf{B} \mid \mathbf{A} \cup \mathbf{Y}) \vee \neg I(\mathbf{X}, \mathbf{Y} \mid \mathbf{A} \cup \mathbf{B}).$$

**Proof** From the decomposition property of conditional independence (Pearl 1988),  $I(\mathbf{X}, (\mathbf{Y} \cup \mathbf{B}) \mid \mathbf{A}) \Rightarrow I(\mathbf{X}, \mathbf{Y} \mid \mathbf{A}) \wedge I(\mathbf{X}, \mathbf{B} \mid \mathbf{A})$  holds. The contraposition of the implication above is  $\neg I(\mathbf{X}, \mathbf{Y} \mid \mathbf{A}) \vee \neg I(\mathbf{X}, \mathbf{B} \mid \mathbf{A}) \Rightarrow \neg I(\mathbf{X}, (\mathbf{Y} \cup \mathbf{B}) \mid \mathbf{A})$ . One obtains

$$\neg I(\mathbf{X}, \mathbf{Y} \mid \mathbf{A}) \Rightarrow \neg I(\mathbf{X}, (\mathbf{Y} \cup \mathbf{B}) \mid \mathbf{A}). \quad (1)$$

From the intersection property of conditional independence (Pearl 1988),  $I(\mathbf{X}, \mathbf{B} \mid \mathbf{A} \cup \mathbf{Y}) \wedge I(\mathbf{X}, \mathbf{Y} \mid \mathbf{A} \cup \mathbf{B}) \Rightarrow I(\mathbf{X}, (\mathbf{Y} \cup \mathbf{B}) \mid \mathbf{A})$  holds. The contraposition of the implication presented above is

$$\neg I(\mathbf{X}, (\mathbf{Y} \cup \mathbf{B}) \mid \mathbf{A}) \Rightarrow \neg I(\mathbf{X}, \mathbf{B} \mid \mathbf{A} \cup \mathbf{Y}) \vee \neg I(\mathbf{X}, \mathbf{Y} \mid \mathbf{A} \cup \mathbf{B}). \quad (2)$$

From (1) and (2), we obtain  $\neg I(\mathbf{X}, \mathbf{Y} \mid \mathbf{A}) \Rightarrow \neg I(\mathbf{X}, \mathbf{B} \mid \mathbf{A} \cup \mathbf{Y}) \vee \neg I(\mathbf{X}, \mathbf{Y} \mid \mathbf{A} \cup \mathbf{B})$ .  $\square$

Consequently, we derive Theorem 3 as explained below.

**Theorem 3** For a sufficiently large sample, the highest BDeu scoring structure consistent with order  $\pi$  is an I-map with the minimum NCP among all the structures consistent with  $\pi$ .

**Proof** We let  $G_\pi^* = (\mathbf{V}, \mathbf{E}_\pi^*)$  be the structure with the highest BDeu among all structures consistent with order  $\pi$ . Also, we let  $G_\pi = (\mathbf{V}, \mathbf{E}_\pi)$  be an arbitrary I-map consistent with  $\pi$ . From the asymptotic consistency of BDeu (Chickering 2002),  $G_\pi^*$  is an I-map. A sufficient condition for Theorem 3 to hold is  $\mathbf{E}_\pi^* \subseteq \mathbf{E}_\pi$ . This proposition can be proved as true by contradiction. Assuming that there exists an I-map consistent with  $\pi$ , denoted as  $G'_\pi = (\mathbf{V}, \mathbf{E}'_\pi)$ , such that  $\mathbf{E}_\pi^* \not\subseteq \mathbf{E}'_\pi$ . This assumption engenders  $\exists X, Y \in \mathbf{V}, (Y \rightarrow X) \in \mathbf{E}_\pi^* \wedge (Y \rightarrow X) \notin \mathbf{E}'_\pi$ . Letting  $\mathbf{A} = \mathbf{Pa}_X^{G_\pi^*} \setminus \{Y\}$ ,

then we obtain  $\neg I(X, Y \mid \mathbf{A})$  from  $(Y \rightarrow X) \in \mathbf{E}_\pi^*$  and the asymptotic local consistency of  $BDeu$  (Chickering 2002). Let  $\mathbf{B}$  be a set of variables  $\text{Pre}_X^\pi \setminus \text{Pa}_{X_0}^{G^*}$ . From  $\neg I(X, Y \mid \mathbf{A})$  and Lemma 1,  $\neg I(X, \mathbf{B} \mid \mathbf{A} \cup \{Y\}) \vee \neg I(X, Y \mid \mathbf{A} \cup \mathbf{B})$  holds, i.e.,  $I(X, \mathbf{B} \mid \mathbf{A} \cup \{Y\}) \Rightarrow \neg I(X, Y \mid \mathbf{A} \cup \mathbf{B})$  holds. Because  $I(X, \mathbf{B} \mid \mathbf{A} \cup \{Y\})$  holds from the local independences in  $G_\pi^*$ , we obtain

$$\neg I(X, Y \mid \mathbf{A} \cup \mathbf{B}). \quad (3)$$

Also,  $D\text{sep}_{G'_\pi}(X, Y \mid \mathbf{A} \cup \mathbf{B})$  holds because  $X$  and  $Y$  are not adjacent in  $G'_\pi$  and because no variable in  $\mathbf{A} \cup \mathbf{B}$  is a descendant of both  $X$  and  $Y$  in  $G'_\pi$ . This result contradicts (3), which completes the proof.  $\square$

Moreover, we derive Theorems 4 and 5 as described below.

**Theorem 4** For any variable set  $\mathbf{V}$ , let  $G^*(\mathbf{V})$  be an I-map with minimum NCP, and let  $G^{NB}(\mathbf{V})$  be the naive Bayes classifiers consisting of a set of feature variables  $\mathbf{V}_c$ , which are children of the class variable in  $G^*(\mathbf{V})$ . The following property holds.

$$NCP(G^{NB}(\mathbf{V}_c)) \leq NCP(G^*(\mathbf{V})).$$

**Proof** Because the parent of feature variables in  $G^{NB}(\mathbf{V}_c)$  is only  $X_0$ , we obtain

$$NCP(G^{NB}(\mathbf{V}_c)) = \sum_{X_i \in \mathbf{V}_c} NCP_i(\{X_0\}) + r_0 - 1,$$

where  $NCP_i(\{X_0\}) = (r_i - 1)r_0$ . For all  $X_i \in \mathbf{V}_c$ , let  $q_i^*$  be the number of parent configurations of  $X_i$  in  $G^*(\mathbf{V})$ . Because  $X_0 \in \text{Pa}_{X_i}^{G^*(\mathbf{V})}$ , we obtain

$$NCP_i(\{X_0\}) \leq NCP_i(\text{Pa}_{X_i}^{G^*(\mathbf{V})}).$$

Consequently, we obtain

$$\begin{aligned} NCP(G^{NB}(\mathbf{V}_c)) &= \sum_{X_i \in \mathbf{V}_c} NCP_i(\{X_0\}) + r_0 - 1 \\ &\leq \sum_{X_i \in \mathbf{V}_c} NCP_i(\text{Pa}_{X_i}^{G^*(\mathbf{V})}) + r_0 - 1 \\ &= NCP(G^*(\mathbf{V})). \end{aligned}$$

$\square$

**Theorem 5**  $h^*$  has consistency.

**Proof** For any pair of nodes  $(\mathbf{U}, \mathbf{R})$  in which  $\mathbf{R}$  has an incoming edge from  $\mathbf{U}$  in an NROG, let  $c(\mathbf{U}, \mathbf{R})$  be a cost of the edge from  $\mathbf{U}$  to  $\mathbf{R}$ . Moreover, let  $X_j$  be a variable included in  $\mathbf{U} \setminus \mathbf{R}$ . When  $X_j \notin \mathbf{V}_c$ , we obtain

$$\begin{aligned} h^*(\mathbf{U}) &= \sum_{X_i \in (\mathbf{U} \cup \mathbf{V}_c)} NCP_i(X_0) \\ &= \sum_{X_i \in (\mathbf{R} \cup \mathbf{V}_c)} NCP_i(X_0) \\ &\leq \sum_{X_i \in (\mathbf{R} \cup \mathbf{V}_c)} NCP_i(X_0) + NCP_j(g_j^*(\mathbf{U} \setminus \{X_j\})) \\ &= h^*(\mathbf{R}) + c(\mathbf{U}, \mathbf{R}). \end{aligned}$$

When  $X_j \in \mathbf{V}_c$ , the following equation holds using  $X_0 \in g_j^*(\mathbf{U} \setminus \{X_j\})$ .

$$\begin{aligned} h^*(\mathbf{U}) &= \sum_{X_i \in (\mathbf{U} \cup \mathbf{V}_c)} NCP_i(X_0) \\ &= \sum_{X_i \in (\mathbf{U} \cup \mathbf{V}_c) \setminus \{X_j\}} NCP_i(X_0) + NCP_j(X_0) \\ &= \sum_{X_i \in (\mathbf{R} \cup \mathbf{V}_c)} NCP_i(X_0) + NCP_j(X_0) \\ &\leq \sum_{X_i \in (\mathbf{R} \cup \mathbf{V}_c)} NCP_i(X_0) + NCP_j(g_j^*(\mathbf{U} \setminus \{X_j\})) \\ &= h^*(\mathbf{R}) + c(\mathbf{U}, \mathbf{R}). \end{aligned}$$

Consequently, we obtain

$$h^*(\mathbf{U}) \leq h^*(\mathbf{R}) + c(\mathbf{U}, \mathbf{R}).$$

$\square$

## References

- Chickering, D. M. 2002. Optimal Structure Identification With Greedy Search. *JMLR*, 3: 507–554.
- Pearl, J. 1988. *Probabilistic Reasoning in Intelligent Systems: Networks of Plausible Inference*. San Francisco, CA, USA: Morgan Kaufmann Publishers Inc. ISBN 1558604790.
- Pearl, J. 2000. *Models, Reasoning, and Inference*. Cambridge University Press.